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13. ABSTRACT *(Maximum 200 words)*

Modeling and computational tools were developed to carry out analyses of dynamic ductile fracture and brittle-ductile transitions without using any ad hoc crack growth criteria. Among the key results obtained were: (i) prediction of a non-monotonic size effect in dynamic ductile failure processes, (ii) resolution of an apparent paradox where under certain loading conditions steels, and other materials, exhibit brittle failure at low loading rates and ductile failure at high loading rates and (iii) three dimensional simulations of dynamic crack growth that, for the first time, illustrate shear lip formation and relate what is seen on the surface with what is happening in the interior, which is generally inaccessible in an experiment. Analyses of deformation and failure in metal-matrix composites revealed that the development of hydrostatic tension fields arising from constrained plastic flow play a key role in determining the deformation and failure behavior of these materials. Detailed comparisons with experiment showed that our analyses provide remarkably accurate predictions of composite behavior and rationalize experimentally observed trends, such as the relative insensitivity of composite yield strength to changes in matrix microstructure and the dependence of ductility on the morphology and distribution of the reinforcement.

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Summary

The aim of the work under this grant was to develop a mechanism based fracture methodology that allows for the possibility of a complete loss of material stress carrying capacity, with the associated creation of new free surface. Hence, fracture, when it occurs, arises as a natural outcome of the loading without any ad hoc failure criterion being employed. Motivation for this stems from the fact that fracture in structures and components is often progressive; local failure causes a redistribution of the stress and deformation fields, which affects the course of subsequent failure, which causes a further stress and deformation redistribution, etc. Accounting for this progression is often essential for predicting final failure.

The modeling and computational tools that we have developed have permitted us to carry out, for the first time, analyses of dynamic ductile crack growth without using any ad hoc crack growth criteria. This provides a physically based continuum mechanics framework for understanding, and hopefully improving, the dynamic toughness of structural metals. Among the key results we have obtained are: (i) prediction of a non-monotonic size effect in dynamic ductile failure processes, (ii) resolution of an apparent paradox where under certain loading conditions steels, and other materials, exhibit brittle failure at low loading rates and ductile failure at high loading rates and (iii) three dimensional simulations of dynamic crack growth that, for the first time, illustrate shear lip formation and relate what is seen on the surface with what is happening in the interior, which is generally inaccessible in an experiment. Our analyses of deformation and failure in metal-matrix composites have revealed that the development of hydrostatic tension fields arising from constrained plastic flow play a key role in determining the deformation and failure behavior of these materials. Detailed comparisons with experiment has shown that our continuum analyses provide remarkably accurate predictions of composite behavior and rationalize experimentally observed trends, such as the relative insensitivity of composite yield strength to changes in matrix microstructure and the dependence of ductility on the morphology and distribution of the reinforcement.

Research Accomplishments

Research under this grant can be divided into the areas of *Analyses of Dynamic Fracture* and *Micromechanical Modeling of Deformation and Failure in Metal Matrix Composites*. An overview of the accomplishments in these two areas is given, but not every research result is described. We note that our work on *3D Modeling of Metallic Fracture* was a Finalist for the 1994 Computerworld-Smithsonian Award in the Science category.

Analyses of Dynamic Fracture

In [4] dynamic crack growth was analyzed numerically for a plane strain double edge cracked specimen subject to symmetric impulsive tensile loading at the two ends. The material behavior is described in terms of an elastic-viscoplastic constitutive model that accounts for ductile fracture by the nucleation and subsequent growth of voids to coalescence using the Gurson constitutive framework. This framework was previously shown to be capable of providing remarkably accurate, quantitative as well as qualitative, descriptions of a variety of ductile failure phenomena. We extended this framework to account for adiabatic heating due to plastic dissipation and the resulting thermal softening. No material length scale is incorporated into this set of constitutive relations. However, a characteristic length can enter the initial/boundary value formulation in a number of other ways. For example, rate sensitive plastic flow together with material inertia gives rise to a characteristic length scale. In our dynamic ductile crack growth analyses, the material length scale represented by the spacing between the larger inclusions has been directly specified, but no length scale is associated with the representation of the smaller inclusions.

Attention in [4] was confined to uniformly spaced large inclusion lying along the initial crack line. Two populations of second phase particles were represented, including large inclusions or inclusion colonies with low strength, which result in large voids near the crack tip at an early stage, and small second phase particles, which require large strains before cavities nucleate. Different prescribed impact velocities, inclusion spacings and values of the inclusion nucleation stress were considered. Predictions for the dynamic crack growth behavior and for the time variation of crack tip characterizing parameters were obtained for each case analyzed. Remarkably, an essentially constant crack speed and constant crack opening angle is predicted for the microstructure analyzed. The spacing between the large inclusions is the key material characteristic length. Doubling the inclusion spacing reduces the crack speed by about 72 percent. The crack growth speed is also sensitive to the specimen size. For a much smaller specimen, where general yielding occurs, much lower crack speeds were found. It is important to emphasize that the crack growth velocities determined in [4] are entirely based on the ductile failure predictions of the material model, and thus are free from ad hoc assumptions regarding appropriate dynamic crack growth criteria.

In [5] a random spacing between large inclusions was considered in order to quantify distribution effects on toughness. A fixed mean spacing characterized each of the six inclusion distributions analyzed. A quantitative measure of the non-uniformity of the distribution is provided by the difference between the mean and the root mean square inclusion spacings. The results indicate that both the COD at the original crack tip needed to grow the crack a fixed amount and the crack speed scale linearly with root mean square inclusion spacing, to a good approximation. Hence, in the circumstances analyzed in [5], resistance to crack growth increases with increasing deviation from uniformity. It may seem contradictory that a non-uniform inclusion distribution increases the resistance to crack growth. For a crack, due to the large gradients of the stress and strain fields near the crack-tip, the interaction and subsequent coalescence of the crack tip with the nearest larger void is a dominant feature of the fracture process. Non-uniform inclusion spacing results in early crack propagation through closely spaced voids, but once the next void near the crack tip has a greater than average spacing further crack propagation requires a load higher than that corresponding to the average spacing. The increased crack growth resistance for a non-uniform inclusion distribution found in the dynamic analyses in [5] is also expected under quasi-static conditions.

In [9] dynamic crack growth along a zig-zag path or a curved path, as is often observed experimentally, was analyzed. Plane strain calculations were carried out for a full edge cracked specimen with various distributions of larger inclusions. A full edge cracked specimen was modeled. For the full specimen, loaded at one end, the stress fields are never symmetric and this non-symmetry together with the inclusion distribution determines the crack path. Remarkably realistic crack growth predictions were obtained. The framework was extended in [17] to model failure by cleavage. The ductile-brittle transition is driven by the fact that the flow strength decreases with decreasing temperature whereas the cleavage stress remains relatively constant. Hence, it is more difficult to achieve the stress levels necessary to initiate cleavage at higher temperatures. The cleavage model in [17] contains a characteristic length scale and involves a spatially non-uniform, but temperature and strain rate independent, critical value of the maximum principal normal stress. The numerical results show a clear transition from cleavage dominated crack growth at low temperatures to purely ductile crack growth at higher temperatures. There is an accompanying increase in the material's resistance to dynamic crack growth. Thus, modeling and computational tools have been developed that provide realistic micromechanical descriptions of both brittle and ductile dynamic crack growth behavior and the transition between these modes.

The influence of material inertia on failure initiation in the round bar tensile test was analyzed numerically in [20]. The material behavior was described in terms of a constitutive relation that models progressive micro-rupture by void nucleation and growth with material strain rate hardening and the thermal softening due to adiabatic heating accounted for. Full dynamic transient analyses were carried out for different sized, geometrically similar specimens, each with a geometric imperfection so that the minimum radius is at the center, and subject to the same nominal strain rate. A critical void volume fraction criteria was used to identify the initiation of failure. Material inertia introduces a length scale so that for fixed material properties and a fixed imposed strain rate, specimen ductility is a function of specimen size. The dependence on specimen size is not monotonic. For sufficiently small specimens, the behavior is much like what would predicted by a quasi-static analysis and is essentially size-independent. As the specimen size is increased, necking and failure are delayed as a consequence of the inertial resistance to motion. Then, for a large enough specimen the deformation inhomogeneity induced by dynamic loading outweighs the initial geometric imperfection and the location of the neck shifts from the specimen center, where the initial cross sectional area is a minimum, to the impact end and the large stresses associated with the loading wave dominate the failure process. Eventually, a specimen size is reached where failure occurs during the initial loading wave and the apparent ductility vanishes. In [20] attention was focused on variations with specimen size at a fixed imposed strain rate. However, similar trends would be expected for a fixed specimen size with the imposed strain rate increasing. Then, for sufficiently small imposed strain rates, the response would be as predicted from a corresponding quasi-static analysis. With increasing strain rate there would at first be an apparent increase in ductility followed by a change in the location of the minimum section and a decrease in apparent ductility.

In [22] the effect of mesh size on the fracture predictions was investigated. Our results showed that the specification of length scales such as inclusion sizes and spacings, and initial crack tip radii, can remove any noticeable mesh sensitivity in the numerical prediction of crack growth, provided the mesh can resolve the local stress and strain gradients at the tip of the growing crack and around the larger voids. Crack growth predictions in cases where the large scale voids dominate had practically no mesh sensitivity, whereas cases dominated by the small scale voids exhibited a clear mesh sensitivity.

In [30] we used a non-local formulation of the constitutive relation for progressive micro-rupture in order to introduce a characteristic length for the small-scale voids. Delocalization is achieved through an integral condition on the rate of increase of the void volume fraction, where the characteristic material length may be considered representative of the average void spacing in the material. Mesh independent results wereobtained in quasi-static analyses of localization and failure showing that this is a possible way of achieving mesh independent failure predictions when the small scale voids dominate the fracture process.

Because of limitations on computational resources, microstructurally based fracture analyses have been carried out using two dimensional plane strain or axisymmetric idealizations. A data parallel formulation was developed in [26] that permits fully three dimensional dynamic ductile failure analyses to be carried out. A key issue in this regard concerns the capability of the numerical implementation to represent plastic flow localization. Strain localization in ductile metals can arise as an inherent outcome of the plastic flow process, e.g. due to yield surface vertex effects or, at high rates of strain, thermal softening, or due to the softening accompanying progressive micro-rupture.

In [26] we carried out full 3D analyses of rectangular cross-section bars subject to dynamic tensile loading using the Gurson constitutive framework for porous plastic solids with elastic-viscoplastic material behavior. This material model allows for the description of void growth to coalescence in a smoothly varying deformation pattern, where the final coalescence stage will often result in localization and fracture, but the model also allows for the prediction of localization in a shear band at an early stage, while the void volume fraction is still small. The 3D transient analyses were carried out using a data parallel numerical implementation that we developed.

The ability of the three dimensional formulation using 20 node brick elements to represent plastic flow localization in shear bands was investigated. For a mesh built up of such higher order elements there will usually not be element boundaries along the characteristic directions for shear bands, and therefore the mesh can only give a diffuse representation of the displacement gradient discontinuity across band interfaces. To test this behavior, a series of three dimensional computations with overall plane strain behavior enforced were carried out, and direct comparison was made with planar studies, where the mesh could be optimally aligned for shear bands. Additionally, a square cross-section tensile test specimen was analyzed for uniaxial loading to investigate the final failure mode in the neck region. Reduced integration lowers the resistance of brick or, in two dimensions, rectangular elements to localized shearing and gives a significant saving in computer time. However, hour-glass instabilities can occur with reduced integration. It was found that the 20 node brick elements with reduced integration were significantly more resistant to hour-glass instabilities than 8 node trilinear brick elements with 1 point quadrature. Thus, the 20 node brick elements with reduced integration were found to represent localization reasonably well, while remaining rather resistant to hour-glass instabilities.

The Charpy V-notch test is a standard laboratory test that is used to obtain a measure of the fracture toughness of materials, and to characterize the brittle-ductile transition. At sufficiently low temperatures fracture in steels and other body centered cubic metals takes place by cleavage, with little absorbed energy, whereas at higher temperatures the fracture mechanism involves ductile hole growth, and much more energy is absorbed. The energy absorbed to fracture in the Charpy test is taken as an indication of the material's toughness. The change from the lower shelf to the

upper shelf on the energy absorption curve defines the transition temperature. In [21] our framework was used to analyze the competition between the ductile and brittle failure mechanisms in Charpy V-notch specimens in a full three dimensional transient analysis.

We found that the initial trends agreed rather well with those expected on the basis of the results for no damage, but as the crack starts to grow from the notch tip, the differences between the three dimensional predictions and the two dimensional plane strain approximation become more noticeable. Thus, particularly in the range of material behavior where cleavage plays an important role a significant amount of crack tunneling develops there was more crack growth at the central part of the notch than near the free edge part of the notch.

Three different levels of flow strength were considered that, for a fixed value of the cleavage stress, spanned most of the brittle-ductile transition, ranging from fully ductile behavior at the upper shelf, with the corresponding high level of energy absorption, to the behavior dominated by brittle cleavage failure near the lower shelf. At the intermediate flow stress level, failure ahead of the central part of the notch occurs by a mixture of the ductile and brittle mechanisms, but even at the highest flow stress analyzed there was an effect of ductile failure, which occurred mainly at the free edge part of the growing crack.

The plane strain computations predicted a force versus time dependence that is initially in rather good agreement with the corresponding three dimensional results, even though the average force level obtained by the two dimensional analysis is a little higher. A planar analysis cannot represent important three dimensional effects, such as the ductile failure region at the free surface edge of a crack growing mainly by the brittle mechanism, or the reduced constraint due to pull-in of the free surface in the notch region, which contributes to much less damping being predicted by the two dimensional plane strain approximation than by a full three dimensional analysis. The time for the onset of cleavage was rather well approximated by the planar analyses, although it was found that these predictions were rather sensitive to the mesh resolution. For all three levels of flow strength considered the plane strain analyses predict more rapid crack growth than found by the three dimensional analyses at the central part of the notch.

Our analyses of brittle-ductile transitions in structural steels under tensile loading in the Charpy V-notch specimen and at the tip of a mode I crack exhibit the usual transition from brittle failure at low temperatures (or high strain rates) to ductile failure at high temperatures (or low strain rates). The mechanism for the brittle-ductile transition can be understood in the following manner; the flow strength decreases with increasing temperature and increases with increasing strain rate. Ductile fracture requires large strains and takes place by the nucleation (from second phase particles), growth and coalescence of voids. Brittle fracture occurs when the stress level is high enough to drive the growth of pre-existing micro-flaws. At high temperatures and low strain rates, plastic flow limits the achievable stress levels so that cleavage does not occur before the large strains needed for ductile fracture are achieved. At lower temperatures or higher strain rates, the stress level required to drive pre-existing micro-cracks can be reached before there is extensive plastic flow and fracture takes place in a brittle manner. Thus, it seemed paradoxical that when Kalthoff impacted steel plates with a cylindrical projectile between two parallel edge cracks, it was observed that at low impact velocities a brittle cleavage fracture occurred, whereas at sufficiently high impact velocities the failure involved shear localization leading to ductile fracture (of course, for low enough impact velocities there is no fracture). This observed fracture mode transition is, of course, exactly the opposite of the usual brittle-ductile transition behavior.

In [28] we carried out a computational simulation of the dynamic shear loading experiment. The calculations show that there are two regions with the greatest straining; directly ahead of the initial crack and at about -135 deg from the initial crack plane. The negative hydrostatic stress below the initial crack plane restricts void growth to the high strain region ahead of the initial crack. The greatest tensile stress is above the initial crack plane. The straining ahead of the initial crack increases more rapidly with impact velocity than does the tensile stress magnitude above the initial crack. Flow localization due to thermal and porosity induced softening can occur, which then reduces the tensile stress magnitude above the initial crack. This is what gives brittle fracture at low impact velocities, and ductile fracture at high impact velocities. The direction of crack propagation, which is quite different for the brittle and ductile failure modes, is also well-predicted by the calculations. The simulations show how the anomalous brittle-ductile transition is related to the mechanics and micro-mechanisms of the fracture process and thus resolve the apparent paradox. It is worth emphasizing that the theoretical framework is the same one that predicts the normal brittle-ductile transition under tensile loading.

Crack growth in structural metals often proceeds by macroscopically flat fracture in the center of a specimen or structure, accompanied by a shear fracture (at an angle of about 45 deg to the internal crack plane) near the free surface. These near surface shear zones are termed "shear-lips." During crack growth only the surface of the specimen is readily accessible, so it is of interest to determine how the surface behavior relates to the internal crack growth. Also, since extensive plastic deformation occurs in the shear-lips, the contribution that the shear-lips make to the apparent ductility is of interest. Shear-lips are a fully three dimensional phenomena so that their simulation requires the 3D computational capability was developed under this grant. In [29] we carried out full three dimensional simulations of dynamic crack growth that, for the first time, illustrate shear lip formation. These simulations related what is seen on the surface with what is happening in the interior, which is generally inaccessible in an experiment and, at best, can only be ascertained after the fact.

Micromechanical Modeling of Deformation and Failure in Metal Matrix Composites

The deformation characteristic of ceramic whisker- and particulate-reinforced metal-matrix composites was studied experimentally and numerically, with the objective of investigating the dependence of mechanical properties on the matrix microstructure and on the size, shape, and distribution of the reinforcement phase. Previous work showed that the development of significant triaxial stresses within the composite matrix, due to the constraint imposed by the reinforcements, gives a major contribution to composite strengthening and apparent strain hardening under monotonic uniaxial loading. In [2] constrained flow of the ductile matrix was shown to lead to the Bauschinger effect in metal-matrix composites, even when the deformation of the matrix is described by isotropic hardening. These results are in qualitative agreement with the experiments in the literature on a 6061 aluminum alloy matrix reinforced with SiC whiskers, thus showing that even when the plastic flow of the matrix material follows an isotropic hardening behavior, the Bauschinger effect is predicted for the composite material. An understanding of the mechanisms responsible for the Bauschinger effect (a tendency for easier plastic flow when the direction of loading is reversed than for continued forward deformation) is necessary for developing constitutive models for complex loading histories and for rationalizing such fatigue phenomena as shakedown and cyclic creep. Furthermore, the ability to predict the Bauschinger effect is often regarded as a test of the validity of strengthening mechanisms because any general theory for strengthening must be capable of rationalizing the deformation behavior upon load reversal.

Deformation and failure of metal-matrix composites, by the nucleation and growth of voids within the metal matrix, were studied numerically and experimentally in [7]. The material systems chosen for parametric analyses and for quantitative comparisons between numerical analyses and experiments were aluminum alloys discontinuously reinforced with SiC. The brittle reinforcement phase, in the form of spheres, particulates with sharp corners, or cylindrical whiskers, was modeled as elastic or rigid, with the interfaces between the ductile matrix and the brittle reinforcement assumed to be perfectly bonded. The matrix material was modeled as an elastic-viscoplastic ductile porous solid to characterize the evolution of damage from void formation. The numerical predictions exhibit trends for the dependence of composite response on reinforcement content, shape and matrix mechanical properties that are in accord with experiment. As in our previous analyses of the monotonic and cyclic response of metal-ceramic composites with fully dense matrices, the hydrostatic stresses that develop due to constrained plastic flow, play a major role in determining the behavior. Quite generally, factors that tend to increase the constraint on plastic flow, tend to decrease the overall strain to matrix failure and vice versa.

The cyclic stress-strain characteristics of discontinuously reinforced metal-matrix composites were investigated both experimentally and numerically in [11]. Two constitutive relations were used to characterize the matrix of the composite, a fully dense Mises solid and the Gurson flow rule for porous plastic solids. The brittle reinforcement phase was modeled as elastic and the interface between the ductile matrix and the reinforcement was presumed to be perfectly bonded. The results provide quantitative information on the evolution of field quantities and ductile failure in the matrix of the composite during fully reversed far-field cyclic loading, on the effects of reinforcement volume fraction and shape on cyclic stress-strain response and failure, on possible mechanisms of cyclic strain-hardening and saturation, and on the effect of the development of matrix porosity on cyclic deformation response. Quantitative predictions of the overall fatigue ductility were also obtained. The development of constraint induced tensile hydrostatic stresses play a major role in influencing cyclic deformation characteristics. While the plastic strains and voids around inclusions are spread throughout the matrix for the particulate composites, they are localized in the vicinity of the reinforcement for the whisker composites. This is a consequence of the fact that particulate composites, with a lower constraint on matrix flow, develop strains that are large enough to induce void nucleation over a significant fraction of the matrix. This prediction of the analysis was supported by experimental observations. The extensive cavitation process mitigates the buildup of tensile hydrostatic stresses that, in turn, slows down void growth. While an increase in the volume fraction of the reinforcement causes an increase in the magnitude of tensile hydrostatic stresses, the resultant elevation in the apparent flow strength can be offset by the nucleation and/or growth of matrix voids. Furthermore, increasing the volume fraction of SiC particulates also promotes higher tensile stresses in the particles and, accordingly, a higher degree of particle fracture. It is worth noting that these aspects of fatigue deformation cannot be quantified solely on the basis of experimental observations.

Many studies of deformation and failure in metal-matrix composites, including the study mentioned above, have been carried out using an isotropic hardening plasticity to characterize the metal matrix. However, SiC whiskers have a diameter of about 0.5 μm, and grain sizes could typically be of comparable size or larger, so that anisotropic crystal slip could have a significant influence on the predicted interaction between matrix deformations and whiskers. Therefore, in [10] and [18] the effect of using crystal plasticity to characterize the matrix was investigated. A planar model of the metal reinforced by short whiskers was used, and results were obtained for three different volume fractions of whiskers. The matrix material was modeled as a single crystal,

allowing for three slip systems. Good agreement between the composite strengthening predicted by continuum slip crystal plasticity and isotropic hardening Mises theory was found.

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